

# Screening at oxide film and nanoparticle surfaces in electrolyte solution by MD simulation

## Scientific Achievement

We have initiated molecular dynamics (MD) simulations of ionic solid-liquid interfaces to elucidate the nature of screening of surface charges in the solid by the surrounding liquid. The ionic solid and liquid are represented by NaCl as a model system interacting via Fumi-Tosi (1964) interionic potential. The liquid is confined between two slabs terminated by (100) surfaces. So as to prevent melting of the slab, its inter-ionic potential has been slightly modified in order to raise its melting point. All the MD simulations are being performed under NVT conditions at three different densities of the NaCl liquid that screens the charges in the slab surface.

The density of the liquid as a function of the distance from the interface exhibits strong layering for highly dense systems (number density = 0.8). The value of static planar structure factor,  $S(\mathbf{k})$ , for the first and second layer in the liquid is 0.78 and 0.55, respectively, indicating strong ionic ordering in the liquid layer next to the interface. Figure 1 shows that this layering disappears rather quickly with decreasing density of the liquid; in fact, already for a number density of 0.6, no layering is observed.

We have also calculated the charge distribution in the liquid as a function of the distance from the interface as seen in Figure 2. In the dense liquid the charge density displays an oscillatory decay, which is a characteristic of screening in dense systems; by contrast, analogous to screening in dilute electrolytes (Debye-Huckel), for a lower density these charge oscillations disappear.

Projected future work involves comparison of computational results on biomolecule-ferroelectric surface interaction with experimental work. Researchers from MSD and ANL Center for Nanoscale Materials researchers have recently started studying bacteriophages expressed via selective binding to  $\text{PbZr}_x\text{Ti}_{1-x}\text{O}_3$  film surfaces, and in the future to  $\text{BaTiO}_3$  surfaces as well.

## Significance

The insights gained from these simulations on the temperature and concentration dependence of the characteristic screening length will help to better understand the self-assembly process of oxide nanoparticles in electrolytic solutions. Our ultimate goal is to develop nanoswitches using amphiphilic block copolymer and ferroelectric surfaces. In these nanoswitches, the electric field direction in the ferroelectric should decide whether the head or tail of the copolymer adsorbs on to the interface. Classical shell-model potentials describing the complex ferroelectric behavior of the barium/strontium titanate system are well developed and published in *J. Phys: Condens. Matter*, **16**, 3495 (2004).

## Performers

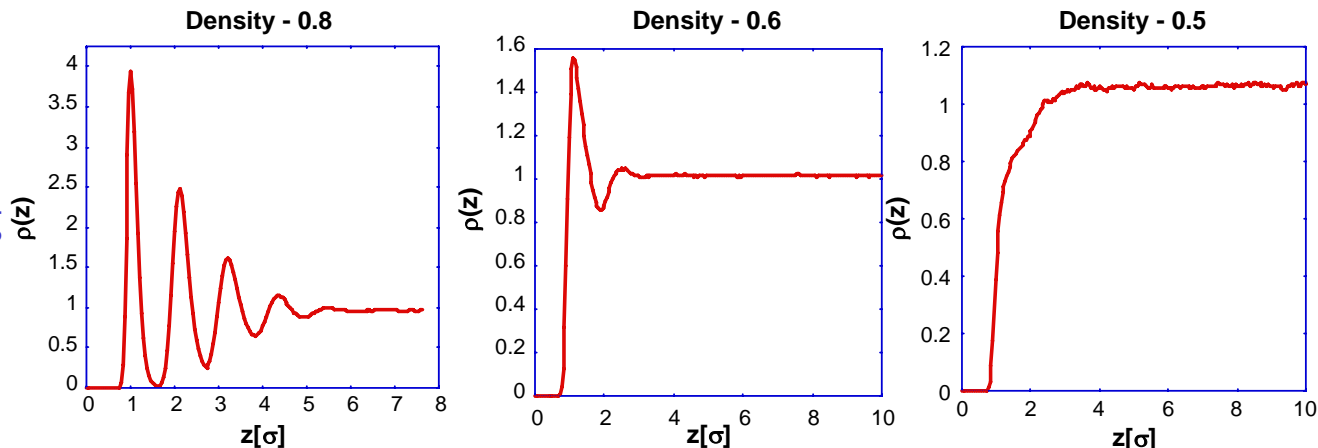
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## Density profile as a function of distance from interface

**Figure 1:**  
*Layering decreases rapidly with decreasing density*



## Charge profile as a function of distance from interface

**Figure 2:**  
*Oscillatory decay of charge density is a characteristic of screening in dense systems*

